Many-body effects on intersubband resonances in narrow InAs/AlSb quantum wells

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Abstract

Intersubband polarization couples to collective excitations of the interacting electron gas confined in a semiconductor quantum well (QW) structure. Such excitations include correlated pair excitations (repellons) and intersubband plasmons (ISPs). The oscillator strength of intersubband resonances (ISBRs) strongly varies with QW parameters and electron density because of this coupling. Using the intersubband semiconductor Bloch equations for a two-conduction-subband model, we show that intersubband absorption spectra for narrow wells are dominated by the Fermi-edge singularity (via coupling to repellons) when the electron gas becomes degenerate and in the presence of large nonparabolicity. Thus, the resonance peak position appears at the Fermi edge and the peak is greatly narrowed, enhanced, and red shifted as compared to the free particle result. Our results uncover a new perspective for ISBRs and indicate the necessity of proper many-body theoretical treatment for modeling and prediction of ISBR line shape.

Key words: Intersubband resonance, Quantum wells, Nonparabolicity, Many-body effects
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1. Introduction

Quantum-well (QW) intersubband resonances (ISBRs) are known to be dressed up by collective excitations [1,2], as a consequence of the Coulomb interaction among the electrons confined in the well, and the dressing renders single particle description of ISBRs insufficient. Early studies showed that coupling to intersubband plasmons (ISPs)—quasiparticles which correspond to coherent superposition of intersubband polarizations—leads to blue shift and narrowing of the ISBRs. This shift is called the depolarization shift. Consequently, it was realized, using density functional theory and self-consistent field theory, that exchange-correlation interaction tends to reduce this blue shift. Later, Nikonov *et al* used Hartree-Fock (HF) approximation and demonstrated that coupling of intersubband polarizations to a light field is drastically modified by the explicit *nonlocal* exchange-interaction-induced vertex correction [2]. Particularly, the exchange inter-

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action strongly alters the way intersubband polarizations couple to each other, leading to appearance of Fermi-edge singularity (FES)-related line shape feature. The FES was studied for interband transitions in a degenerate semiconductor [3], where the Mahan exciton was introduced. Compared to the interband case, repellons exist in intersubband transitions [2], due to negative reduced mass. Repellons are un-bound collective excitations and temperature sensitive. Therefore, for ISBRs, the polarizations couple to both ISPs and repellons. Strictly speaking, we do *not* see pure repellon or ISP—we have a mixed excitation, which, as limiting cases, recovers the two collective excitations.

In ISBR studies in the framework of self-consistent field theory [4], only dynamical coupling to ISPs was considered, which allows depolarization shift and narrowing of the ISBRs in the presence of nonparabolicity (dispersive energy difference between ground subband and the excited subband—a source of inhomogeneous line broadening). With vertex correction included in the presence of nonparabolicity, there is a redistribution of the oscillator strength, which depends upon QW thickness and electron density. It is then interesting to see the interplay of the two types of collective excitations [5]. We adopted the Hartree-Fock approach [6,7] to set up the intersubband semiconductor Bloch equations for a two-conduction-subband model. Systematic investigations were done with material parameters (nonparabolicity, for example), electron variables (both density and temperature), and quantitative comparison with InAs/AlSb QW measurements [8,9]. Here we report a model study for narrow wells that illustrates that intersubband absorption spectra are dominated by FES (repellons) when the electron gas becomes degenerate and in the presence of strong nonparabolicity. We lay out our theoretical considerations and equations in the following section, followed by simulation results and discussions in Sec. 3. We conclude in Sec. 4.

2. Theoretical Model

In the framework of the Hartree-Fock approximation, many-body effects on ISBRs are due to (i) self-energy correction to the single particle energy, (ii) vertex correction to the electric field an electron experiences, and (iii) an additional correction to the electric field an electron experiences because of dynamic screening from the other electrons. The first two contributions come from exchange interaction (Fock term), whereas the last one is from the direct Coulomb interaction (Hartree term). The first contribution renormalizes the single particle energy, whereas the other two contributions lead to the so-called *local field* correction to the light electric field. Higher order correlations were ignored in the present study–they introduce additional contributions, like screening by the exchange interaction, and tend to modify the above first-order contributions . Dephasing, caused by these higher order correlations, was modeled with a constant rate.

The QW growth is along the $\hat{\boldsymbol{z}}$ direction. The equation of motion was derived for dynamic variable $f_{mn}(\boldsymbol{k})$ ($\equiv \langle c^{\dagger}_{m\boldsymbol{k}} c_{n\boldsymbol{k}} \rangle$, which means taking the average of quantum transition from state $|n\boldsymbol{k}\rangle$ to $|m\boldsymbol{k}\rangle$ over the canonical quantum ensemble of the system), where m or $n = 1, 2$ for ground ($= 1$) and excited subband ($= 2$), and $\boldsymbol{k}$ is the in-plane wave vector. In a two-subband model, $f_{11}(\boldsymbol{k})$ ($f_{22}(\boldsymbol{k})$) is the electron distribution function for the ground (excited) subband; $p(\boldsymbol{k}) \equiv f_{12}(\boldsymbol{k})$ is the intersubband polarization function. The resultant equations are termed the intersubband semiconductor-Bloch equations and given below:

$$\dot{f}_{11}(\boldsymbol{k}) = -\mathcal{I}m[2\Omega_{\boldsymbol{k}} p(\boldsymbol{k})] + \dot{f}_{11}(\boldsymbol{k})|_{inc}, \tag{1}$$

$$\dot{f}_{22}(\boldsymbol{k}) = \mathcal{I}m[2\Omega_{\boldsymbol{k}} p(\boldsymbol{k})] + \dot{f}_{22}(\boldsymbol{k})|_{inc}, \tag{2}$$

$$\dot{p}(\boldsymbol{k}) = (\varepsilon_{2\boldsymbol{k}} - \varepsilon_{1\boldsymbol{k}})p(\boldsymbol{k})/i\hbar + i\Omega_{\boldsymbol{k}}[f_{11}(\boldsymbol{k}) - f_{22}(\boldsymbol{k})] + \dot{p}(\boldsymbol{k})|_{inc} \ , \tag{3}$$

where a dot on top of a quantity stands for the time derivative of that quantity, $\Omega_{\boldsymbol{k}} = [\boldsymbol{d}_{\boldsymbol{k}} \cdot \boldsymbol{E}_{\perp}(t) - \varepsilon_{21\boldsymbol{k}}]/\hbar$ is the generalized Rabi frequency, $\varepsilon_{m\boldsymbol{k}} = E_m(\boldsymbol{k}) + \varepsilon_{mm\boldsymbol{k}}$ is the renormalized electron energy consisting of subband dispersion (first term) and self-energy (second term), $\boldsymbol{d}_{\boldsymbol{k}}$ is the electric dipole matrix element ($\hat{\boldsymbol{z}}$ component only for TM light field), and $\varepsilon_{21\boldsymbol{k}}$ is the local field correction contribution. The local field effect has two Coulomb sources: a vertex correction reflecting the nonlocal nature of exchange interaction, and a depolarization term arising from dynamic screening due to direct Coulomb interaction among electrons. The vertex term is responsible for a repellon-like resonance, whereas the depolarization term introduces ISP-like response. The terms with subscript *inc* represent electron-electron and electron-LO phonon scatterings [7], which were substituted with a constant—relaxation time approximation. Modeling detail will be separately published [8].

In the linear response regime for ISBRs, the electron distributions were given by the Fermi function, and the intersubband polarization equation (3) was linearized with respect to the light field. Then, we applied the rotating wave approximation and made an ansatz $p(\boldsymbol{k}) = P_{\boldsymbol{k}} \exp(-i\omega t)$ for the incident light field $\boldsymbol{E}_{\perp}(t) = E_0 \exp(-i\omega t)\hat{\boldsymbol{z}}$. Under these treatments, Eq. (3) was reduced to the following form:

$$[\hbar(\omega + i\gamma_p) - (\varepsilon_{2\boldsymbol{k}} - \varepsilon_{1\boldsymbol{k}})]\, P_{\boldsymbol{k}} = (d_{\boldsymbol{k}} E_0 - \varepsilon_{21\boldsymbol{k}})(f_{22\boldsymbol{k}} - f_{11\boldsymbol{k}}) \; , \tag{4}$$

where γ_p is the constant dephasing rate. We used numerical matrix inversion to solve the above equation and obtain $P_{\boldsymbol{k}}$. Then, the susceptibility was found according to $\chi(\omega) \equiv P/\varepsilon_0 E_0$ with the total polarization P given by $2S/[(2\pi)^2\mathcal{V}] \int d\boldsymbol{k} d^*_{\boldsymbol{k}} P_{\boldsymbol{k}}$, where $\mathcal{V} = WS$, W is the QW thickness and S is a normalization area. The theoretical absorbance is approximately given by $\omega W\, \mathcal{I}m\,[\chi(\omega)]\,/nc$. n is the background refractive index and c is the speed of light in vacuo.

3. Numerical Results and Discussions

As input to Eq. (4), the subband dispersion was assumed to be parabolic, *i.e.*, $E_m(\boldsymbol{k}) = E_m^{(0)} + \hbar^2 \boldsymbol{k}^2/2m_m$ with the confinement energy $E_m^{(0)}$ and the effective masses determined with the quantum box model, together with all QW form factors used in simulating ISBR spectra. (Note that different effective masses in the subbands model nonparabolicity of the system in an approximate way. Nonparabolicity arises from both the bulk band structure and the heterogeneous nature of the QW structure.) We used $m_1 = 0.027 m_e$, $m_2 = 0.039 m_e$, $d_{\boldsymbol{k}} = 31\ e.\mathring{A}$. m_e is free electron mass. The dephasing rate γ_p was taken to be 1 meV. The single plasmon pole approximation was used for screening [6]. We chose an electron density of 1×10^{12} cm^{-2} and temperature of 12 K so that the electron gas is degenerate. All other input parameters are standard. To better reveal the FES behavior introduced by the vertex correction, the QW thickness was chosen to be very small ($W = 16\ \mathring{A}$) such that influence of the depolarization field is reduced to a negligible level, as will be seen in the simulated spectra.

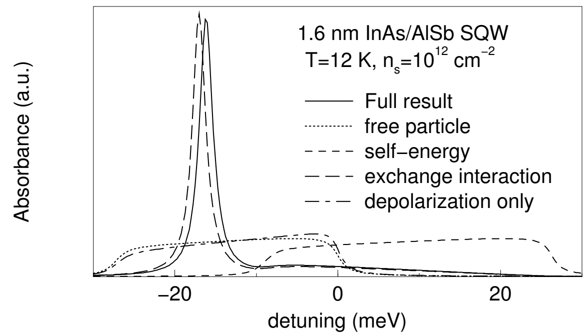

Fig. 1. Absorbance for a narrow single quantum well with large nonparabolicity. For comparison, part of, or whole many-body contributions were purposely switched off to illustrate the individual effects: “Full result” kept all contributions (solid line); “free particle” had no many-body contributions (dotted line); “self-energy” included only exchange self-energy (dashed line); “exchange interaction” neglected depolarization field (long dashed line); and “depolarization only” considered only depolarization field (dot-dashed line).

The results, shown in Fig. 1, are striking. Quite the opposite from what a theory without vertex correction would predict (as shown by the “depolarization only” curve), the absorbance features a strong resonance near the Fermi energy. As mentioned, many-body effects on ISBRs are due to self-energy, vertex correction, and a depolarization field. To identify different roles these contributions play, we intentionally switched part of, or all contributions off. The “free particle” spectrum, as a reference, was calculated without any Coulomb contributions. As seen, it exhibits the fermionic nature of electrons: phase-space filling to the Fermi level, which is only observable in the presence of nonparabolicity. The flat-top line broadening over 20 meV reflects the 2D nature of the phase space and severe degree of nonparabolicity in InAs. After the self-energy is added, the spectrum is blue shifted by about 20 meV because the energy of the occupied ground subband is lowered while the empty excited subband is not affected. (Note that the Fermi edge in ISBR spectrum is also blue shifted accordingly as it corresponds to the low energy end of the spectrum.) Because this energy lowering is momentum-dependent, the spectrum is further flattened and broadened. The spectrum takes a drastic transformation after vertex correction is switched on:

a rather sharp resonance (long dashed line in Fig. 1). The reason is simple: there exists a large degree of cancellation of the effects by self-energy and vertex correction. It can be shown from Eq. (3) that in the total polarization equation, these two terms cancel out [2], but the equation is not closed in the presence of nonparabolicity. The resonance in this case stands for excitation of the repellons by the light field, despite the fact that such repellons are unstable. In contrast, the “depolarization only” spectrum, with only the direct Coulomb (Hartree) interaction, shows a negligible deviation from the “free particle” one. The effect by the depolarization field is negligible because (i) the characteristic number for measurement of strength of the depolarization field is only 0.04 [2], and (ii) the presence of large nonparabolicity in InAs makes excitation of the intersubband plasmon—coherent superposition of intersubband polarizations—less favorable owing to inhomogeneous broadening. It would need a relatively thick QW and high electron density to approach the limiting case of excitation of the plasmons. Therefore, it is not surprising now, after including all the Coulomb contributions, that the “Full result” closely resembles the spectrum with exchange interaction only. The depolarization field slightly blue shifts the spectrum relative to the FES result. This shows unambiguously that ISBRs are dominated by the Coulomb interaction, which leads to collective excitations. Within a certain parameter window, the collective excitations are of the FES nature.

4. Concluding Remarks

Our intersubband semiconductor Bloch equations-based model allows a more systematic study of many-body effects on quantum-well intersubband absorption spectra. In particular, we report here that for very narrow wells (thus much weakened depolarization effect), intersubband resonances are dominated by Fermi-edge singularity via coupling to repellons when the electron gas is degenerate and in the presence of large nonparabolicity. As a result, the resonance appears at the Fermi edge, largely narrowed, enhanced, and red shifted as compared to the free particle result. The revelation strengthens the viewpoint of the Coulomb interaction-dominated nature of intersubband resonances. The study shows the importance of interplay of collective excitations on shaping the absorption spectra.

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